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DB=USPT; PLUR=YES; OP=OR

L24 L23 and (l13) 1 L24

L23 L22 and (symmetry axes) 25137 L23

L22 (fusion protein and oligomerization domain) 212421 L22

DB=PGPB; PLUR=YES; OP=OR

L21 L19 and (axis) 1 L21

L20 L19 and (axes) 1 L20

L19 20070218547 1 L19

DB=USPT; PLUR=YES; OP=OR

L18 6756039.pn. 1 L18

L17 L14 and l13 0 L17

L16 L15 and l14 0 L16

L15 colovos.in. 4 L15

L14 yoshida.in. 11698 L14

L13 padilla.in. 176 L13

<u>L12</u>	yeastes.in.	0	<u>L12</u>
<u>L11</u>	L1 and (homodimeric or homotetrameric)	0	<u>L11</u>
<u>L10</u>	L1 and (covalent bond)	0	<u>L10</u>
<u>L9</u>	L1 and (non-intersecting axes)	0	<u>L9</u>
<u>L8</u>	L1 and (linker)	1	<u>L8</u>
<u>L7</u>	L1 and (influenza virus)	1	<u>L7</u>
<u>L6</u>	L1 and (oligomerization domain)	1	<u>L6</u>
<u>L5</u>	L1 and (tetrameric or dimeric structure)	1	<u>L5</u>
<u>L4</u>	6242570.pn.	1	<u>L4</u>
<u>L3</u>	5877279.pn.	1	<u>L3</u>
<u>L2</u>	5573925.pn.	1	<u>L2</u>
<u>L1</u>	5008373.pn.	1	<u>L1</u>

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NEWS	4	JUL 02	CHEMCATS accession numbers revised
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NEWS	6	JUL 16	CAplus enhanced with French and German abstracts
NEWS	7	JUL 18	CA/Capplus patent coverage enhanced
NEWS	8	JUL 26	USPATFULL/USPAT2 enhanced with IPC reclassification
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NEWS	16	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data
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NEWS	18	SEP 13	FORIS renamed to SOFIS
NEWS	19	SEP 13	INPADOCDB enhanced with monthly SDI frequency
NEWS	20	SEP 17	CA/Capplus enhanced with printed CA page images from 1967-1998
NEWS	21	SEP 17	CAplus coverage extended to include traditional medicine patents
NEWS	22	SEP 24	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS	23	OCT 02	CA/Capplus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS	24	OCT 19	BEILSTEIN updated with new compounds
NEWS EXPRESS	19	SEPTEMBER 2007:	CURRENT WINDOWS VERSION IS V8.2, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.
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=> s fusion protein and (homodimeric or homotetrameric)
6 FILES SEARCHED...

L1 4505 FUSION PROTEIN AND (HOMODIMERIC OR HOMOTETRAMERIC)

=>

=> s l1 and (geometry)
L2 171 L1 AND (GEOMETRY)

=> s l2 and (covalent bond)
L3 17 L2 AND (COVALENT BOND)

=> s l3 and (oligomerization domains)
L4 4 L3 AND (OLIGOMERIZATION DOMAINS)

=> d l4 ti abs ibib tot

L4 ANSWER 1 OF 4 USPATFULL on STN

TI Self assembling proteins for producing extended materials

AB Self-assembling fusion proteins and nucleic acids encoding the same are provided. The subject fusion proteins include a first dimer forming oligomerization domain and a second tetramer forming oligomerization domain rigidly linked to each other. Also provided are regular structures made up of a plurality of self-assembled fusion proteins of the subject invention, and methods for producing the same. The subject fusion proteins find use in the preparation of self-assembled nanostructures, e.g., two-dimensional layers and three-dimensional networks, which structures find use in a variety of different applications.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

ACCESSION NUMBER: 2007:249911 USPATFULL

TITLE: Self assembling proteins for producing extended materials

INVENTOR(S): Yeates, Todd O., Agoura Hills, CA, UNITED STATES
Padilla, Jennifer, Pasadena, CA, UNITED STATES
Yoshida, Stephanie, Seattle, WA, UNITED STATES
Colovos, Chris, Thousand Oaks, CA, UNITED STATES

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2007218547	A1	20070920
APPLICATION INFO.:	US 2004-815543	A1	20040331 (10)
RELATED APPLN. INFO.:	Continuation-in-part of Ser. No. US 2000-564710, filed on 3 May 2000, GRANTED, Pat. No. US 6756039		

	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-133470P	19990510 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	BOZICEVIC, FIELD & FRANCIS LLP, 1900 UNIVERSITY AVENUE, SUITE 200, EAST PALO ALTO, CA, 94303, US	
NUMBER OF CLAIMS:	26	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	1 Drawing Page(s)	
LINE COUNT:	611	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

L4 ANSWER 2 OF 4 USPATFULL on STN

TI Adzymes and uses thereof

AB Disclosed is a family of novel protein constructs, useful as drugs and for other purposes, termed "adzymes," comprising an address moiety and a catalytic domain. In some types of disclosed adzymes, the address binds with a binding site on or in functional proximity to a targeted biomolecule, e.g., an extracellular targeted biomolecule, and is disposed adjacent the catalytic domain so that its affinity serves to confer a new specificity to the catalytic domain by increasing the effective local concentration of the target in the vicinity of the catalytic domain. The present invention also provides pharmaceutical compositions comprising these adzymes, methods of making adzymes, DNA's encoding adzymes or parts thereof, and methods of using adzymes, such as for treating human subjects suffering from a disease, such as a disease associated with a soluble or membrane bound molecule, e.g., an allergic or inflammatory disease.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

ACCESSION NUMBER: 2005:87403 USPATFULL

TITLE: Adzymes and uses thereof

INVENTOR(S): Afeyan, Noubar B., Lexington, MA, UNITED STATES
Lee, Frank D., Chestnut Hill, MA, UNITED STATES
Wong, Gordon G., Brookline, MA, UNITED STATES
Das Gupta, Ruchira, Auburndale, MA, UNITED STATES
Baynes, Brian, Somerville, MA, UNITED STATES
PATENT ASSIGNEE(S): COMPOUND THERAPEUTICS, INC., Waltham, MA (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2005074865	A1	20050407
APPLICATION INFO.:	US 2004-792498	A1	20040302 (10)
RELATED APPLN. INFO.:	Continuation-in-part of Ser. No. US 2003-650592, filed on 27 Aug 2003, PENDING		

	NUMBER	DATE
PRIORITY INFORMATION:	US 2002-406517P	20020827 (60)
	US 2002-423754P	20021105 (60)
	US 2002-430001P	20021127 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	FISH & NEAVE IP GROUP, ROPES & GRAY LLP, ONE INTERNATIONAL PLACE, BOSTON, MA, 02110-2624	
NUMBER OF CLAIMS:	45	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	25 Drawing Page(s)	
LINE COUNT:	9195	
CAS INDEXING IS AVAILABLE FOR THIS PATENT.		

L4 ANSWER 3 OF 4 USPATFULL on STN

TI Adzymes and uses thereof

AB Disclosed is a family of novel protein constructs, useful as drugs and for other purposes, termed "adzymes," comprising an address moiety and a catalytic domain. In some types of disclosed adzymes, the address binds with a binding site on or in functional proximity to a targeted biomolecule, e.g., an extracellular targeted biomolecule, and is disposed adjacent the catalytic domain so that its affinity serves to confer a new specificity to the catalytic domain by increasing the effective local concentration of the target in the vicinity of the catalytic domain. The present invention also provides pharmaceutical compositions comprising these adzymes, methods of making adzymes, DNA's encoding adzymes or parts thereof, and methods of using adzymes, such as for treating human subjects suffering from a disease, such as a disease associated with a soluble or membrane bound molecule, e.g., an allergic or inflammatory disease.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

ACCESSION NUMBER: 2004:107249 USPATFULL

TITLE: Adzymes and uses thereof

INVENTOR(S): Afeyan, Noubar B., Lexington, MA, UNITED STATES
Lee, Frank D., Chestnut Hill, MA, UNITED STATES
Wong, Gordon G., Brookline, MA, UNITED STATES
Das Gupta, Ruchira, Auburndale, MA, UNITED STATES
Baynes, Brian, Somerville, MA, UNITED STATES

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2004081648	A1	20040429
APPLICATION INFO.:	US 2003-650592	A1	20030827 (10)

	NUMBER	DATE
PRIORITY INFORMATION:	US 2002-406517P	20020827 (60)
	US 2002-423754P	20021105 (60)
	US 2002-430001P	20021127 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	ROPES & GRAY LLP, ONE INTERNATIONAL PLACE, BOSTON, MA, 02110-2624	
NUMBER OF CLAIMS:	156	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	19 Drawing Page(s)	
LINE COUNT:	8325	
CAS INDEXING IS AVAILABLE FOR THIS PATENT.		

L4 ANSWER 4 OF 4 USPATFULL on STN

TI Adzymes and uses thereof

AB Disclosed is a family of novel protein constructs, useful as drugs and

for other purposes, termed "adzymes," comprising an address moiety and a catalytic domain. In some types of disclosed adzymes, the address binds with a binding site on or in functional proximity to a targeted biomolecule, e.g., an extracellular targeted biomolecule, and is disposed adjacent the catalytic domain so that its affinity serves to confer a new specificity to the catalytic domain by increasing the effective local concentration of the target in the vicinity of the catalytic domain. The present invention also provides pharmaceutical compositions comprising these adzymes, methods of making adzymes, DNA's encoding adzymes or parts thereof, and methods of using adzymes, such as for treating human subjects suffering from a disease, such as a disease associated with a soluble or membrane bound molecule, e.g., an allergic or inflammatory disease.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

ACCESSION NUMBER: 2004:107248 USPATFULL
 TITLE: Adzymes and uses thereof
 INVENTOR(S): Afeyan, Noubar B., Lexington, MA, UNITED STATES
 Lee, Frank D., Chestnut Hill, MA, UNITED STATES
 Wong, Gordon G., Brookline, MA, UNITED STATES
 DasGupta, Ruchira, Auburndale, MA, UNITED STATES
 Baynes, Brian, Somerville, MA, UNITED STATES

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2004081647	A1	20040429
APPLICATION INFO.:	US 2003-650591	A1	20030827 (10)

	NUMBER	DATE
PRIORITY INFORMATION:	US 2002-406517P	20020827 (60)
	US 2002-423754P	20021105 (60)
	US 2002-430001P	20021127 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	ROPES & GRAY LLP, ONE INTERNATIONAL PLACE, BOSTON, MA, 02110-2624	
NUMBER OF CLAIMS:	41	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	19 Drawing Page(s)	
LINE COUNT:	7919	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

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E2      1      YEATERWILLIAMS M/AU
E3     119 --> YEATES/AU
E4      51      YEATES A/AU
E5      45      YEATES A E/AU
E6      10      YEATES A J/AU
E7       5      YEATES A N/AU
E8       4      YEATES A P/AU
E9       3      YEATES A R/AU
E10     85      YEATES A T/AU
E11     12      YEATES A TODD/AU
E12     22      YEATES ALAN T/AU
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L5      12 "YEATES A TODD"/AU
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L5 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN

TI Nonlinear Optical Transmission and Multiphoton Processes in Organics IV.
(Proceedings held 14-15 August 2006 in San Diego, California.) [In: Proc.
SPIE-Int. Society Opt. English; 2006, 6330]
AB Unavailable
ACCESSION NUMBER: 2007:5660 HCAPLUS
DOCUMENT NUMBER: 146:71450
TITLE: Nonlinear Optical Transmission and Multiphoton
Processes in Organics IV. (Proceedings held 14-15
August 2006 in San Diego, California.) [In: Proc.
SPIE-Int. Society Opt. English; 2006, 6330]
AUTHOR(S): Yeates, A. Todd; Belfield, Kevin D.; Kajzar,
Francois; Editors
CORPORATE SOURCE: USA
SOURCE: (2006) Publisher: (SPIE-The International Society for
Optical Engineering: Bellingham, Wash.), No pp. given.
ISBN: 0-8194-6409-0
DOCUMENT TYPE: Book
LANGUAGE: English

L5 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN

TI Nonlinear Optical Transmission and Multiphoton Processes in Organics III.
(Proceedings held in San Diego, CA 2 August 2005.) [In: Proc. SPIE-Int.
Society Opt. English, 2005; 5934]
AB Unavailable
ACCESSION NUMBER: 2005:1282015 HCAPLUS
DOCUMENT NUMBER: 144:42874
TITLE: Nonlinear Optical Transmission and Multiphoton
Processes in Organics III. (Proceedings held in San
Diego, CA 2 August 2005.) [In: Proc. SPIE-Int. Society
Opt. English, 2005; 5934]
AUTHOR(S): Yeates, A. Todd; Editor
CORPORATE SOURCE: USA
SOURCE: (2005) Publisher: (SPIE-The International Society for
Optical Engineering: Bellingham, Wash.), No pp. given.
ISBN: 0-8194-5939-9
DOCUMENT TYPE: Book
LANGUAGE: English

L5 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN

TI Nonlinear optical ionic liquids

AB A review. MO calcns. indicate that mols. with a high electron d. diffused
over a large volume will have third order nonlinear optical activity.
Anions often have higher second hyperpolarizability values (γ) than
similar neutral mols. Also, mols. or ions containing higher row elements have
higher γ s. Salts with cations that have their pos. charge only weakly
interacting with the anion also enhance the third order nonlinear optical
activity. That looks like the recipe for ionic liqs. A number of
sulfur-containing mono- and dianion salts were synthesized and characterized
through Z-scan measurements. Most were ionic liqs., and some showed
significant third order nonlinear optical behavior. The general features
of ionic liqs. such as wide liquidus range, good thermal stability, and
low vapor pressure are particularly advantageous for applications of
nonlinear optical materials. Potential applications are in optical
limiting and other all optical devices.

ACCESSION NUMBER: 2005:683430 HCAPLUS
DOCUMENT NUMBER: 143:305727
TITLE: Nonlinear optical ionic liquids
AUTHOR(S): Del Sesto, Rico E.; Dudis, Doug S.; Ghebremichael,
Fassil; Heimer, Norman E.; Low, Tammy K. C.; Wilkes,
John S.; Yeates, A. Todd
CORPORATE SOURCE: Department of Chemistry, U.S. Air Force Academy,
Colorado Springs, CO, 80840, USA
SOURCE: ACS Symposium Series (2005), 902(Ionic Liquids IIIB:
Fundamentals, Progress, Challenges, and

Opportunities), 144-158
CODEN: ACSMC8; ISSN: 0097-6156
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN
TI Proceedings of SPIE Conference on Nonlinear Optical Transmission and
Multiphoton Processes in Organics held 3-4 August 2003 in San Diego,
California. [In: Proc. SPIE-Int. Society Opt. English, 2003; 5211]
AB Unavailable
ACCESSION NUMBER: 2004:229410 HCAPLUS
DOCUMENT NUMBER: 141:215300
TITLE: Proceedings of SPIE Conference on Nonlinear Optical
Transmission and Multiphoton Processes in Organics
held 3-4 August 2003 in San Diego, California. [In:
Proc. SPIE-Int. Society Opt. English, 2003; 5211]
AUTHOR(S): Yeates, A. Todd; Belfield, Kevin D.; Kajzar,
Francois; Lawson, Christopher M.; Editors
CORPORATE SOURCE: USA
SOURCE: (2003) Publisher: (SPIE-The International Society for
Optical Engineering: Bellingham, Wash.), 148 pp.
ISBN: 0-8194-5084-7
DOCUMENT TYPE: Book
LANGUAGE: English

L5 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN
TI Nonlinear optical ionic liquids
AB MO calcns. indicate that mols. with a high electron d. diffused over a
large volume will have third order nonlinear optical activity. Anions often
have higher second hyperpolarizability values (γ) than similar neutral
mols. Also, mols. or ions containing higher row elements have higher γ s.
Salts with cations that have their pos. charge only weakly interacting
with the anion also enhance the third order nonlinear optical activity.
That looks like the recipe for ionic liqs. A number of sulfur-containing mono-
and dianion salts were synthesized and characterized through Z-scan
measurements. Most were ionic liqs., and some showed significant third
order nonlinear optical behavior. The general features of ionic liqs.
such as wide liquidus range, good thermal stability, and low vapor
pressure are particularly advantageous for applications of nonlinear
optical materials. Potential applications are in optical limiting and
other all-optical devices.
ACCESSION NUMBER: 2003:632567 HCAPLUS
TITLE: Nonlinear optical ionic liquids
AUTHOR(S): Wilkes, John S.; Del Sesto, Rico E.; Ghebremichael,
Fassil; Heimer, Norman E.; Dudis, Douglas S.;
Yeates, A. Todd
CORPORATE SOURCE: Department of Chemistry, US Air Force Academy, USAF
Academy, CO, 80840-6230, USA
SOURCE: Abstracts of Papers, 226th ACS National Meeting, New
York, NY, United States, September 7-11, 2003 (2003),
IEC-088. American Chemical Society: Washington, D. C.
CODEN: 69EKY9
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English

L5 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN
TI Parallel computational chemical calculations for Air Force material
projects
AB We will report results on two chemical systems of interest to the Air Force:
C122 complexes and Pt-containing oligomers. The former are excellent electron
acceptors, while the latter have interesting non-linear optical

properties. It is known that C122 complexes, which are two buckminsterfullerene (C60) balls connected by an acetylene bridge, are good electron acceptors: the AM1 electron affinity is of the order of 8 eV. In order to characterize these mols. more fully, we have performed calcns., at the generalized gradient approximation level of DFT, studying the bridging found in these compds. These can be characterized as vertex, 5-6 edge, or 6-6 edge bridging. We have characterized the HOMO and LUMO orbitals for the various neutral conformations, as well as for anionic species. Trans-bis(acetylene phenyl)bis(tri Bu phosphine)Pt has been synthesized in our labs. Several derivative oligomers have also been synthesized and their visible spectrum has been characterized. We have performed ab initio DFT calcns. to try to provide insight on the ground state and the low lying excited states in order to provide insight onto the non-linear optical properties of these mols.

ACCESSION NUMBER: 2003:631201 HCAPLUS
TITLE: Parallel computational chemical calculations for Air Force material projects
AUTHOR(S): Blaudeau, Jean-Philippe; Dudis, Douglas S.; Yeates, A. Todd; Cooper, Thomas M.
CORPORATE SOURCE: ASC/HP, High Performance Computing Inc, Wright-Patterson Air Force Base, OH, 43235, USA
SOURCE: Abstracts of Papers, 226th ACS National Meeting, New York, NY, United States, September 7-11, 2003 (2003), COMP-041. American Chemical Society: Washington, D. C.
CODEN: 69EKY9
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English

L5 ANSWER 7 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN
TI Cisoid defects in all-trans polyenes and polyacetylene
AB Polyacetylene is the paradigm of conjugated materials and is of key importance for its electronic, optical, and nonlinear optical properties. Obtaining samples of defect-free polyacetylene is hampered by the ready formation of various types of defects in the polymer backbone. The formation of cisoid defects within an all-trans polyene, and in the long limit, all trans-polyacetylene, has been studied by means of Hartree-Fock and correlated (second order perturbation theory) ab initio calcns. In the present contribution we report the results obtained for a series of all trans-polyenes of general formula C_nH_{n+2} , $n=4, 8, 12, \dots, 28$. Each mol. in this series possesses a central carbon-carbon single bond about which rotation is feasible. The rotation barrier for each member of this series has been determined, as well as the optimized trans-cisoid metastable structure, vibrational properties and structural changes as a function of chain length. Extrapolation of these properties as they evolve into the infinite limit yields the description of the trans-cisoid defect in t-PA. Surprisingly, the extended conjugation results in a rather low rotation barrier, which can be understood from increasing ease of electron manipulation (polarization). SCF calcns. predict a non-planar defect, whereas inclusion of correlation yields a planar defect.

ACCESSION NUMBER: 2003:182040 HCAPLUS
TITLE: Cisoid defects in all-trans polyenes and polyacetylene
AUTHOR(S): Dudis, Doug S.; Ryan, James J.; Yeates, A. Todd
CORPORATE SOURCE: Polymer Group, Air Force Research Laboratory, Wright-Patterson AFB, OH, 45433, USA
SOURCE: Abstracts of Papers, 225th ACS National Meeting, New Orleans, LA, United States, March 23-27, 2003 (2003), COMP-354. American Chemical Society: Washington, D. C.
CODEN: 69DSA4
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English

L5 ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN

TI Raman responses of cis- and trans-polyenes

AB Recent reports of exceptionally large Raman responses in low-defect trans-polyacetylene (Kobryanskii polyacetylene) have prompted speculations regarding the origin of such large signals. We have applied correlated (post-Hartree Fock) calcns. on an extensive series polyenes to investigate the origin of these responses. Two important conclusions are (1) all trans-polyenes, in the absence of defects, have tremendous Raman responses which are orders of magnitude larger than some standard, highly Raman-active materials, and (2) no special mechanisms need be invoked to explain such responses. Conventional mechanisms are adequate to account for the large responses.

ACCESSION NUMBER: 2003:182039 HCAPLUS

TITLE: Raman responses of cis- and trans-polyenes

AUTHOR(S): Yeates, A. Todd; Dudis, Doug S.

CORPORATE SOURCE: Materials & Manufacturing Directorate, Air Force Research Laboratory, Wright-Patterson AFB, OH, 45433-7750, USA

SOURCE: Abstracts of Papers, 225th ACS National Meeting, New Orleans, LA, United States, March 23-27, 2003 (2003), COMP-353. American Chemical Society: Washington, D. C.

CODEN: 69DSA4

DOCUMENT TYPE: Conference; Meeting Abstract

LANGUAGE: English

L5 ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN

TI Electron affinities and Jahn-Teller distortions in C60 anions

AB Buckminsterfullere, C60, is well known to be highly electron-accepting, undergoing up to six (6) successive one-electron redns. under certain conditions. The high electron affinity of C60 is important for mol.-electronic technologies, such as photovoltaics, while the geometric distortions of the various anions are crucial to understanding electron-phonon coupling in various superconductive fullerenes. Surprisingly, full ab initio gradient-optimized structures have not been reported for many if not most of the various anions to the best of our knowledge. Herein we report full SCF (Hartree-Fock) as well as hybrid d. functional (B3LYP) calcns. in an effort to map the structure-charge-multiplicity landscape at theories that treat electron-electron interactions consistently from one state to another.

ACCESSION NUMBER: 2003:181711 HCAPLUS

TITLE: Electron affinities and Jahn-Teller distortions in C60 anions

AUTHOR(S): Dudis, Doug S.; Yeates, A. Todd; Blaudeau, Jean-Philippe

CORPORATE SOURCE: Polymer Group, Air Force Research Laboratory, Wright-Patterson AFB, OH, 45433, USA

SOURCE: Abstracts of Papers, 225th ACS National Meeting, New Orleans, LA, United States, March 23-27, 2003 (2003), COMP-024. American Chemical Society: Washington, D. C.

CODEN: 69DSA4

DOCUMENT TYPE: Conference; Meeting Abstract

LANGUAGE: English

L5 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN

TI Concepts and modeling approaches in conjugated materials.

AB Abstract text not available.

ACCESSION NUMBER: 2000:794559 HCAPLUS

TITLE: Concepts and modeling approaches in conjugated materials.

AUTHOR(S): Dudis, Douglas S.; Yeates, A. Todd

CORPORATE SOURCE: AFRL/MLBP, Wright Research Laboratory, Wright Patterson AFB, OH, 45433, USA

SOURCE: Abstracts of Papers, 220th ACS National Meeting,
Washington, DC, United States, August 20-24, 2000
(2000) COMP-050
CODEN: 69FZC3
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal; Meeting Abstract
LANGUAGE: English

L5 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN

TI Polymer ionization energies and electron affinities: Polyacetylene.
AB The calcn. of polymer electronic properties has presented tremendous challenges both theor. and computationally. The introduction of the singlet-triplet method as a viable approach to model polymer band-gaps provides tremendous insight into electronic processes in polymeric systems. In particular, the inclusion of electron-electron interactions, especially those terms considered in the self consistent field theories, are critical to obtaining qual. and quant. correct answers. Simple HOMO-LUMO approaches, which neglect half the problem, are not adequate. In the present work the electron affinity and ionization energy of ideal polyacetylene is determined from calcns. on a variety of oligomers. Post-Hartree Fock correlation is also considered in terms of bounding the problem.

ACCESSION NUMBER: 1999:540719 HCAPLUS
TITLE: Polymer ionization energies and electron affinities:
Polyacetylene.
AUTHOR(S): Dudis, Douglas S.; Yeates, A. Todd
CORPORATE SOURCE: Materials & Manufacturing Directorate, Air Force
Research Laboratory, Wright-Patterson AFB, OH,
45433-7750, USA
SOURCE: Book of Abstracts, 218th ACS National Meeting, New
Orleans, Aug. 22-26 (1999), COMP-009. American
Chemical Society: Washington, D. C.
CODEN: 67ZJA5
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English

L5 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2007 ACS on STN

TI Prediction of third-order NLO properties of organic molecules
AB A review with >19 refs. on the calcn. of γ values and structural effects on γ .

ACCESSION NUMBER: 1994:629997 HCAPLUS
DOCUMENT NUMBER: 121:229997
TITLE: Prediction of third-order NLO properties of organic molecules
AUTHOR(S): Dudis, Douglas S.; Yeates, A. Todd; Kost, Daniel
CORPORATE SOURCE: Department of Chemistry, Ben Gurion University, Beer Sheva, 84105, Israel
SOURCE: Advanced Materials (Weinheim, Germany) (1994), 6(3), 248-51
CODEN: ADVMEW; ISSN: 0935-9648
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English